Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information: Kinetic-energy-based error quantification in Kohn-Sham density functional theory

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Table S1 Various density error metrics for molecular systems, including normed integral absolute deviations in densities, density gradients, and density Laplacians; normed absolute errors in non-interacting kinetic energies; and normed deviations in the total energy evaluated using Kohn-Sham and Hartree-Fock densities as inputs to corresponding Kohn-Sham energy functional.